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AN APPROXIMATE MODEL WITH CHEMICAL REACTION FOR A THERMOELECTRIC PLANT GAS RELEASED

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Abstract. *The problem of air pollution, the spread of the emitted gases and impacts to the environment have drawn attention. The spread of gases emitted from a thermal power plant with coal burning, is presented in this work. The flow of the chimney are described by "AP-42" - Compilation of Emission Factors for Air Pollutants from the "Environmental Protection Agency (EPA)" of the United States. A computer program is being developed and was used to describe the source of emission and propagation of gases. The approximate model separates the propagation mechanism (advection and diffusion) and chemical reaction. A simplified chemical mechanism separating the chemistry of gases Nitrogen (NOx) and volatile organic compounds ("VOC") is discussed. Numerical results are presented for the concentrations of the gases emitted from this chimney.*

Keywords: *Propagation; gas dispersion, chemical reactions.*

1. INTRODUCTION

In the recent decades, air pollution has drawn attention because of their harmful effect on the environment. The study of the dispersion and transport of gases in the atmosphere has attracted the attention of many research groups. One of the sources of emissions is industrial smokestacks, Fenger (1999). These gases may undergo chemical transformations in the atmosphere to produce products that will interact with the environment. For example, Sulfur Oxides (SOx) and nitrogen (NOx) are precursors to acid rain and Nitrogen Dioxide (NO_2) gas produces ozone present in the lower atmosphere, Seinfeld and Pandis (2006). The spread of the gases emitted from a thermal power plant coal, is represented by an approximate model. This work describes the model of propagation, dispersion and chemical reaction. Also shown are the numerical results obtained for the concentrations of gases Nitric acid (HNO3), Nitrogen Dioxide (NO2), nitrous oxide (NO) and ozone (O3) generated from the emission source downwind.

2. APPROXIMATE MODEL OF SPREAD WITH CHEMICAL REACTION

2.1 Source Emission of the Coal Thermal Power Plant

The main gases involved with smog NOx, SOx, carbon monoxide (CO) and Volatile Organic Compounds (VOCs) have their flow rates estimated from emission factors inventory "AP-42", USEPA (). The flow rates of the gases leaving the chimney are estimated by the relation:

$$Q_{i,E} = A_i \times E_{F,i} \times (1 - \frac{E_{R,i}}{100}) \quad (1)$$

Where Q_i is the flow rate of the compound "i" (kg h-1) obtained by emission factors, A_i is the rate of fuel consumption (kg h-1), $E_{F,i}$ is the emission factor for gas " i "(kg gas" i "/ kg total) and $E_{R,i}$ is the elimination factor of the gas in the pollution removal equipment. The other gas flow rates are determined by stoichiometry ratios, the amount of excess air employed and elemental analysis of the Candiota Coal shown in Table 1, according to Rodrigues (2004). The amount of gas generated per each kg of coal from each element present in the coal, for example, carbon dioxide (CO_2) is obtained from the element Carbon (C) is obtained by the following equation

$$(X_{gi})_C = \frac{\bar{M}_{gi}}{\bar{M}_i}(X_i)_{um}) \quad (2)$$

Where $(X_{gi})_C$ is the amount of gas "gi" in kg per kg of coal, M_{gi} is the molar mass of the gas coming out the chimney and M_i is the molar mass of the element "i" that reacts with oxygen. The flow, the other gases, are given by the relation

$$Q_{i,D} = (X_{gi})_C A_i \quad (3)$$

Where $Q_{i,D}$ is the flow of other gases.

Table 1. Elementary data of the coal.

Compounds	% of the mass fraction
H_2O	3.58
Volatile material	19.77
Fixed Carbon	25.66
Ash	54.57
Sulfur	2.04
Carbon	32.26
Hydrogen	2.13
Nitrogen	0.67
Oxygen + halogen	8.33

2.2 Propagation Model with Chemical Reaction

The propagation model (advection, dispersion and chemical reaction) of exhaust gases from the chimney adopts an instant release (so-called "puff") of rectangular shape, which separates the chemical reaction mechanisms and propagation at each liberation time of the "puff ", as Orlandi (2004). The chemical reaction model adopts the variation of the concentration of the gas mixture at a constant volume of the "puff", at each released time. And, the propagation model is an approximate model that applies to dilution of the total mass of gas released at the end of the travel time. The standard uses a dilution solution of the diffusion equation for the propagation of the total mass of gases to evaluate the inlet every time offset. These models are presented below.

2.2.1 Simplified Model of Chemical Reactions for obtaining HNO_3

In this work we adopted a simplified model for the evaluation of the nitric acid formed in the atmosphere from nitrogen compounds released in Thermal Power Plant. The set of reactions was uncoupled reactions of Volatile Organic Compounds (VOC) for an evaluation of the results and ease of solution of the set of ordinary differential equations that have numerical instability problem, as Yamartino et al. (1992). The set of reactions used is shown:

1) $NO_2 + h\nu \xrightarrow{O_2} NO + O_3$ $\quad R_1 = J_1 C_{NO_2}$

2) $O_3 + h\nu \rightarrow O_2 + O'$ $\quad R_2 = J_2\ C_{O_3}$

3) $O_3 + NO \rightarrow NO_2 + O_2$ $\quad R_3 = k_3 C_{O_3} C_{NO}$

4) $H_2O + O' \rightarrow 2OH$ $\quad R_4 = k_4 C_{H_2O} C_{O'}$

5) $OH + NO_2 \rightarrow HNO_3$ $\qquad R_5 = k_5 C_{OH} C_{NO_2}$

This set of reactions origins the following set of ordinary differential equations that describe the mass balance in a system of constant volume for gases,

$$\frac{dC_{NO_2}}{dt} = -J_1 C_{NO_2} + k_3 C_{NO} C_{O_3} - k_5 C_{NO_2} C_{OH} \quad (4)$$
$$\frac{dC_{NO}}{dt} = J_1 C_{NO_2} - k_3 C_{NO} C_{O_3} \quad (5)$$
$$\frac{dC_{O_3}}{dt} = J_1 C_{NO_2} - J_2 C_{O_3} - k_3 C_{NO} C_{O_3} \quad (6)$$
$$\frac{dC_{O'}}{dt} = J_2 C_{O_3} - k_4 C_{O'} C_{H_2O} \quad (7)$$
$$\frac{dC_{H_2O}}{dt} = -k_4 C_{O'} C_{H_2O} \quad (8)$$
$$\frac{dC_{OH}}{dt} = 2k_4 C_{O'} C_{H_2O} - k_5 C_{NO_2} C_{OH} \quad (9)$$
$$\frac{dC_{HNO_3}}{dt} = k_5 C_{NO_2} C_{OH} \quad (10)$$
$$\frac{dC_{O_2}}{dt} = -J_1 C_{NO_2} + J_2 C_{O_3} + k_3 C_{O_2} C_{NO} \quad (11)$$

2.2.2 Model of Chemical Reactions

The system of seven equations ordinary coupled to the seven components, describes the mass balance of the components of the chemistry of HNO3 in a constant volume, this is handled independent of the atmospheric dispersion (dilution with atmospheric air). The system is solved at each "puff" displacement time by the method implicit numerical integration "Backward Differentiation Formula" fourth order BDF

$$y_n = \frac{48}{25} y_{n-1} - \frac{36}{25} y_{n-2} + \frac{16}{25} y_{n-3} - \frac{3}{25} y_{n-4} + h \frac{12}{25} f(y_n, t_n) \quad (12)$$

Where y_n is the value of the function at time "t_n", h is the integration step number f (y_n, t_n) is the derivative function of y calculated at the present time. The integration step is a very small value due to the problems of rigidity, the difference of reaction rates of the components, faster reactions and slow reactions. The discretization generates a non-linear system of equations for the concentrations. It is solved by the method of successive substitution at every step of integration.

2.2.3 The model advection and dispersion of the "puff"

The instantaneous release is approximated by a model of homogeneous properties, called box models, as Seinfeld and Pandis (2006). It adopted the shape of a prism with a rectangular base for this "puff", according to Figure 1. A local solution of the diffusion equation is used to determine the concentration profile and the air intake to the "puff".

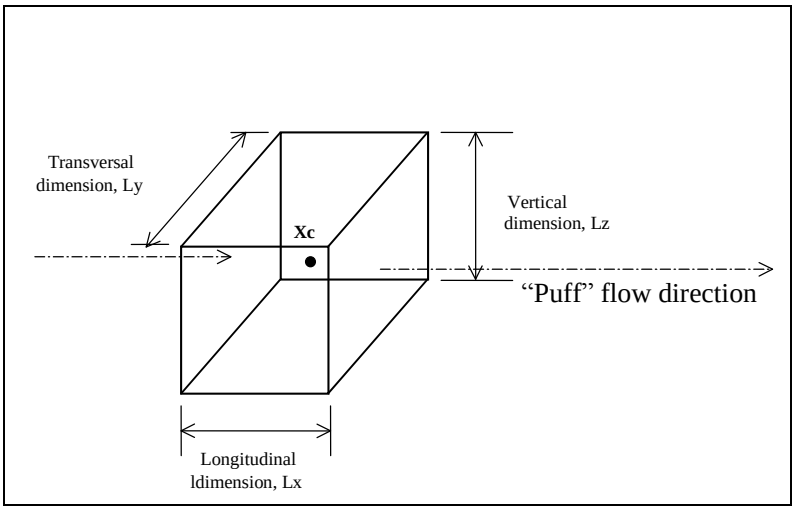

Figure 1 - "Puff" prism with rectangular base.

The "puff" contains the following variables that characterize it: the total mass of gas (m_{gp}), the position of its center relative to the emission source (XC_i) the longitudinal dimension ($L_{x,i}$) the transverse ($L_{y,i}$), the vertical dimension ($L_{z,i}$), the travel time in the atmosphere (t_p), and the total release time from the source (t_t).

The volume of the gas "puff" is determined by:

$$V_i = L_{x,i} L_{y,i} L_{z,i} \tag{13}$$

Where i refers to the total time "i".

The total concentration of all the gases in the "puff" is given by the relationship:

$$\rho_{gp,i} = \frac{m_{gp,i}}{L_{x,i} L_{y,i} L_{z,i}} \tag{14}$$

Where $\rho_{gp,i}$ is the total concentration of the “puff” i.

The position of the center "puff" is determined for each time displacement of the "puff" by:

$$x_{C,i} = x_{C,i-1} + u_{m,i} t_p \tag{15}$$

Where $X_{C,i}$ is the position of the center of the "puff", $u_{m,i}$ is the average speed of the "puff" (obtained from the average logarithmic velocity profile) and the time t_p displacement of the "puff".

The travel time of the "puff" has been adopted equal to the release time of the emission source which is the ratio of the mass of the released gas in the source by flow rate of the gas

$$t_p = \frac{m_{gp,0}}{Q} \tag{16}$$

The "puff" of gas includes a quantity of air, at each displacement time, and has its dimensions adjusted by the relations:

$$\boldsymbol{L_{x,i} = L_{x,i-1} + \Delta x_i} \tag{17}$$
$$\boldsymbol{L_{y,i} = L_{y,i-1} + \Delta y_i} \tag{18}$$
$$\boldsymbol{L_{z,i} = L_{z,i-1} + \Delta z_i} \tag{19}$$

Where Δ x, Δ y Δ z are the increases in the longitudinal, transverse and vertical directions, respectively.

2.2.4 The inlet model of the air for the “puff”

The variation of the concentration of the components in the "puff" due to diffusion of components in the atmosphere is evaluated with a new procedure from the atmospheric air inlet to its interior. The mean total mass of gas "puff" with the time offset is given by:

$$\boldsymbol{\rho_{gp,m} = \frac{m_{gp}}{V_{i-1} + \Delta V_i}} \tag{20}$$

Where $\rho_{gp,m}$ is the average of the total concentration of the "puff", V_i is the volume of the anterior "puff" and ΔV_i is the volume of air that entered to the "puff" at the time of displacement. Then, the volume of intake air is determined from the average concentration

$$\Delta V_i = \frac{m_{gp} - \rho_{gp,m} V_{i-1}}{\rho_{gp,m}} \tag{21}$$

This procedure connects the approximate model of "puff" rectangular with a particular solution of the diffusion equation for the total emission.

The expression for estimating the concentration of the Gaussian plume at a point of coordinates (x, y, z) is given by

$$\rho_{pl} = \frac{Q}{2\pi u_{m,i}\sigma_{y,i}\sigma_{z,i}} e^{-\left[\frac{y^2}{2\sigma_{y,i}^2}\right]} \left(e^{\left[\frac{-(z-h)^2}{2\sigma_{z,i}^2}\right]} + e^{\left[\frac{-(z+h)^2}{2\sigma_{z,i}^2}\right]} \right) \quad (22)$$

Where ρ_{pl} is the concentration at the point (x, y, z), Q is the flow rate of the source, $u_{m,i}$ is the average wind speed, $\sigma_{y,i}$ is the coefficient of atmospheric dispersion in the transverse direction, $\sigma_{z,i}$ is the coefficient of atmospheric dispersion in the vertical direction, y is the transverse direction to point source, z is the vertical direction of the point source and h is the height of the chimney.

The mean of the Gaussian plume in the region of dimensions ($L_{x,i}$, $L_{y,i}$ and $L_{z,i}$) is given by

$$\rho_{gp,m} = \frac{Q\,\mathrm{erf}\left(\frac{L_{y,i}}{2\sqrt{2}\sigma_y}\right)\left[\mathrm{erf}\left(\frac{L_{z,i}}{2\sqrt{2}\sigma_z}\right)+\frac{1}{2}\mathrm{erf}\left(\frac{2h+\frac{L_{z,i}}{2}}{\sqrt{2}\sigma_z}\right)-\frac{1}{2}\mathrm{erf}\left(\frac{2h-\frac{L_{z,i}}{2}}{\sqrt{2}\sigma_z}\right)\right]}{u_i L_{y,i} L_{z,i}} \quad (23)$$

The new dimensions of the "puff" rectangle are determined from the amount by volume of air that enters at each interval. This procedure connects the approximate model of "puff" rectangular with a particular solution of the diffusion equation for the total emission.

The dimensions are derived from an approximation of the ratio between the dimensions "puff" and the atmospheric dispersion coefficients in the time shift:

$$\frac{\Delta x_i}{\Delta z_i} = \frac{0{,}2\sigma_{x,i}}{\sigma_{z,i}} \quad (24)$$

$$\frac{\Delta y_i}{\Delta z_i} = \frac{\sigma_{y,i}}{\sigma_{z,i}} \quad (25)$$

$$\Delta V_i = (L_{x,i} + \Delta x_i)(L_{y,i} + \Delta y_i)(L_{z,i} + \Delta z_i) - L_{x,i} L_{y,i} L_{z,i} \quad (26)$$

3. METHODOLOGY

The methodology used was to apply the model described. It was implemented in a computer program in Fortran, with free software plus Force Fortran 90. The program makes the readings of the characterization data of the coal, the source of emission, atmospheric composition and characteristics of the wind and weather runs propagation model with chemical reaction.

4. RESULTS OBTAINED FROM THE MODEL

The model was applied to an emission source, according to data cited by the company CGTEE (2012) for the phase called "B", on a sunny day and the characteristics of unstable atmosphere. These data are shown in Table 2. The results are shown in Figures 2 to 6. The graphs show concentration values in the ordinate against the distance from the emission point on the axis of abscissa. Figures 2 and 3 show the concentration of gas Nitrogen Dioxide (NO2) from the release into the chimney (0 m) to that of Figure 5 and Figure 6 nitrous oxide to the nitric acid. Figure 4 shows the input volume of air per dilution. Figure 7 shows the concentration of nitrogen compounds on the same graph. This figure shows the behavior of the reagent NO_2, of the reaction intermediates NO and of the reaction product HNO_3.

Table 2. Parameters used in the simulation.

Source emission data	
Flow rate, in kg s^{-1}	0.275560
chimney height, in m	150.0
Chimney diameter, in m	5.0
Atmosphere data	
Atmospheric pressure, in atm	1.0
Temperature, in ^oC	25.0
Air relative humidity, in %	30.0
Wind speed at 10 m, in m s^{-1}	7.0
Convective velocity, in m s^{-1}	1.64
Convective boundary layer length, in m	780.0

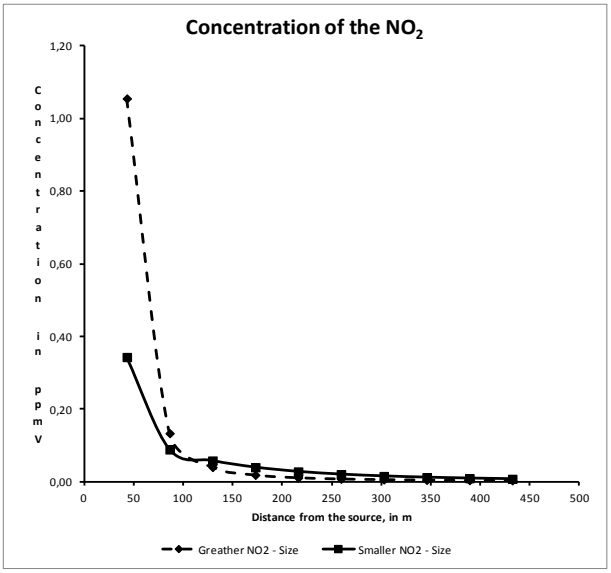

Figure 2. NO_2 concentration profile of the distance 0 to 400 m.

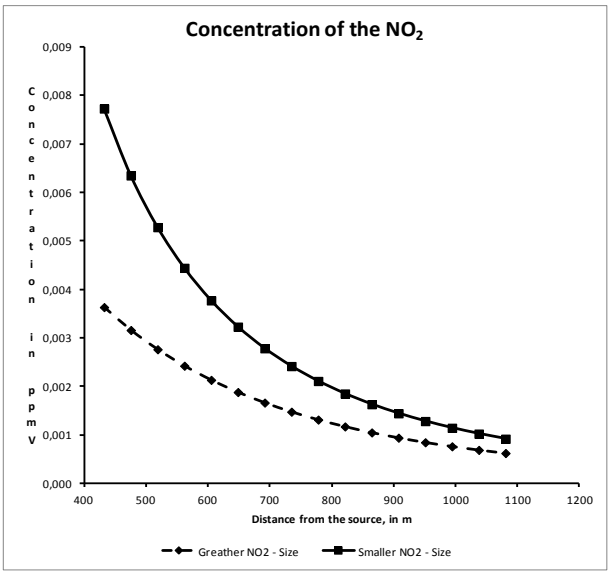

Figure 3. NO2 concentration profile of 400-1100 m.

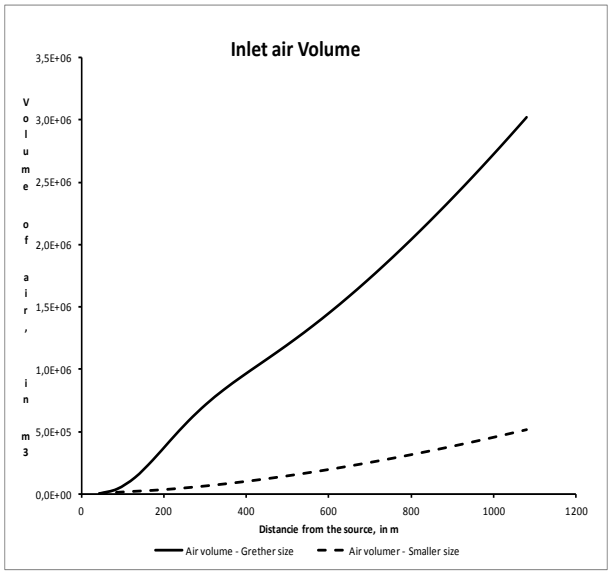

Figure 4. Volume of intake air by diffusion.

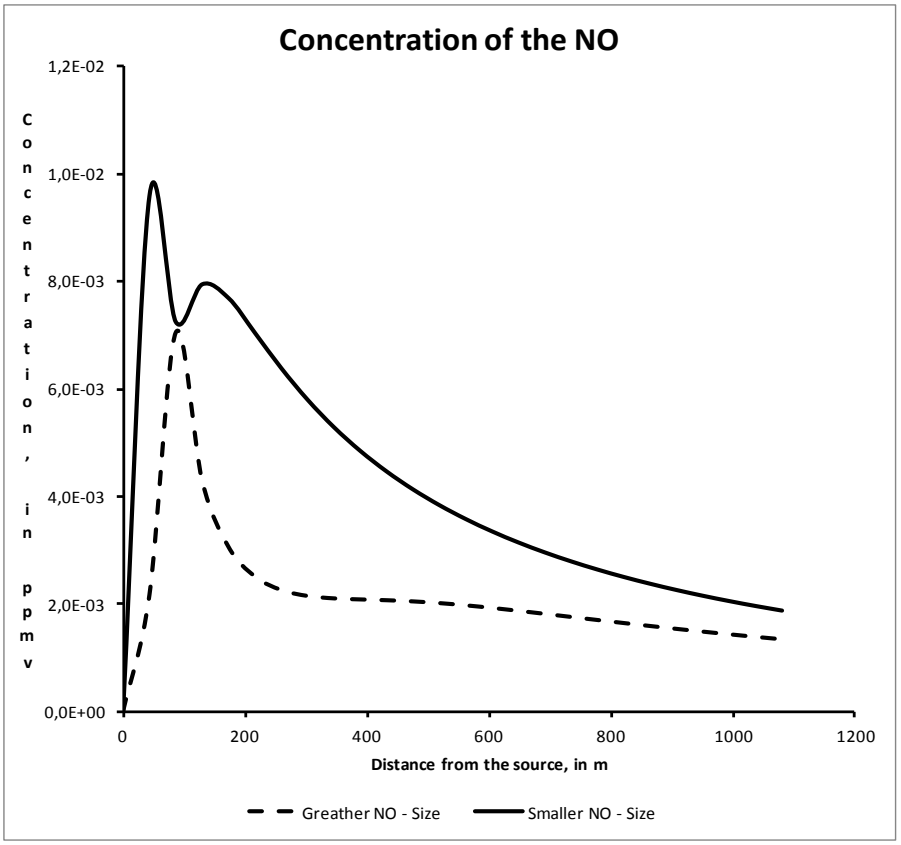

Figure 5. NO concentration profile to a distance of 1100 m.

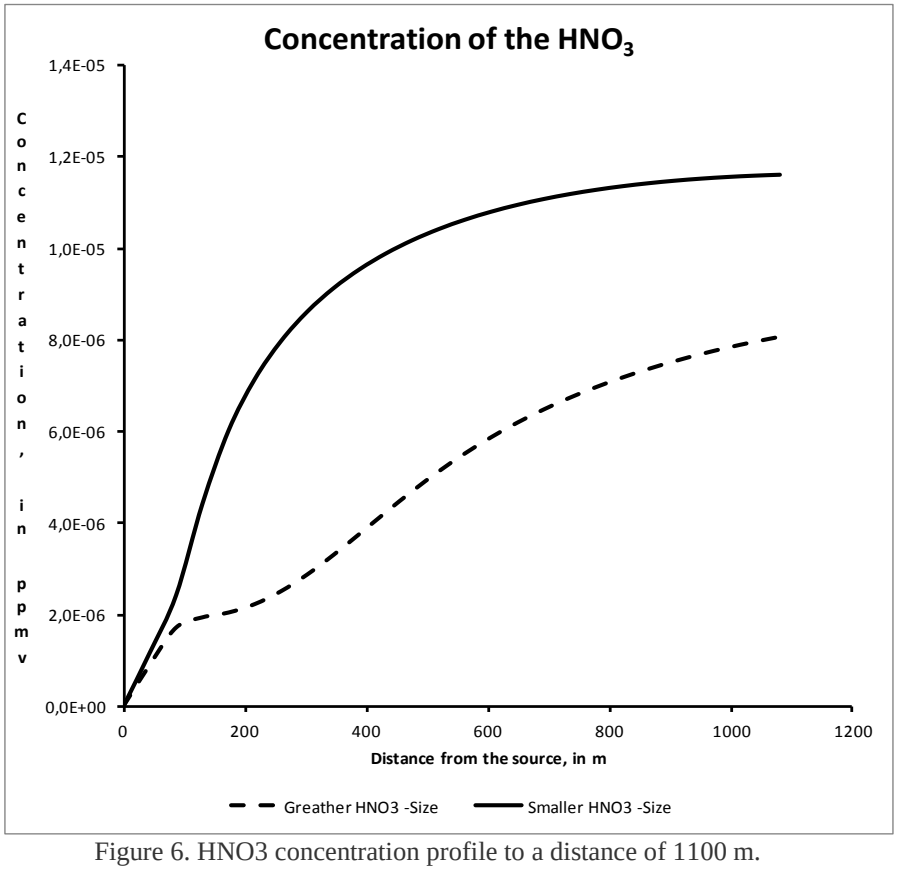

Figure 6. HNO3 concentration profile to a distance of 1100 m.

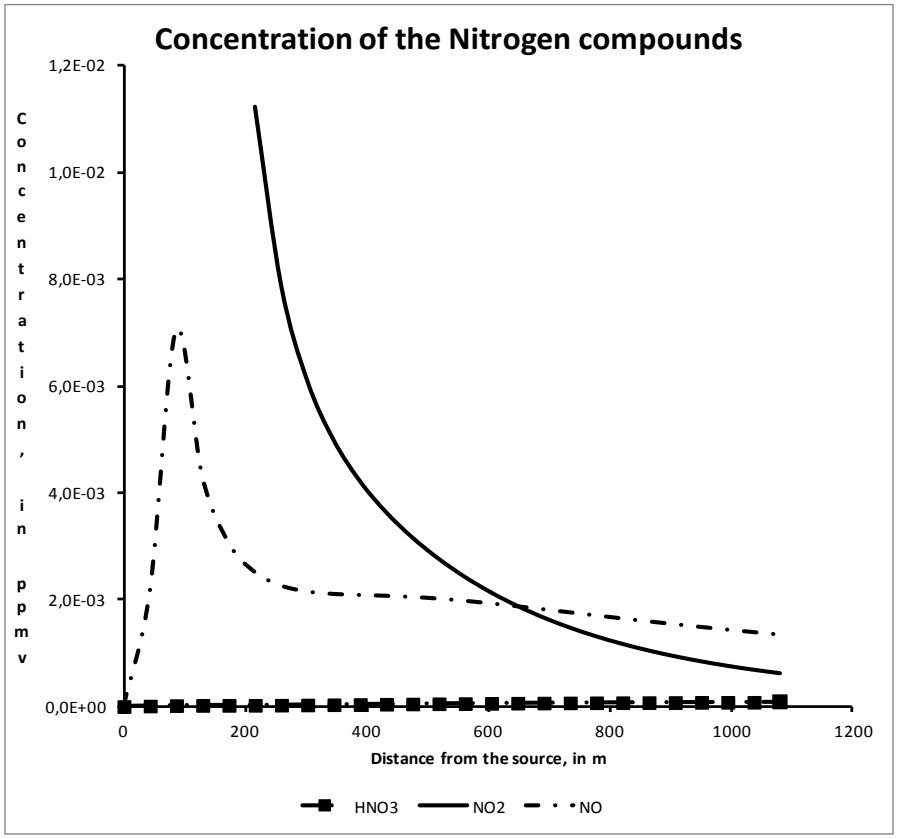

Figure 7. Concentration profile of nitrogen compounds.

5. CONCLUSIONS

This model approximate separating the dispersion mechanisms and overall chemical reaction is adequate because the solution becomes faster. The model will be developed further and more applications are performed.

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